

# Thulium nickel/lithium distannide, $\text{TmNi}_{1-x}\text{Li}_x\text{Sn}_2$ ( $x = 0.035$ )

Andrij Stetskiv,<sup>a</sup> Ivan Tarasiuk,<sup>b\*</sup> Renata Misztal<sup>c</sup> and  
Volodymyr Pavlyuk<sup>b,c</sup>

<sup>a</sup>Ivano-Frankivsk National Medical University, Department of Chemistry, Galyska str. 2, 76018 Ivano-Frankivsk, Ukraine, <sup>b</sup>Department of Inorganic Chemistry, Ivan Franko Lviv National University, Kyryla and Mefodiya str. 6, 79005 Lviv, Ukraine, and <sup>c</sup>Institute of Chemistry, Environment Protection and Biotechnology, Jan Dlugosz University, al. Armii Krajowej 13/15, 42-200 Czestochowa, Poland  
Correspondence e-mail: tarasiuk.i@gmail.com

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Key indicators: single-crystal X-ray study;  $T = 293$  K; mean  $\sigma(\text{Sn-Ni}) = 0.002$  Å; disorder in main residue;  $R$  factor = 0.026;  $wR$  factor = 0.060; data-to-parameter ratio = 17.2.

The quaternary thulium nickel/lithium distannide,  $\text{TmNi}_{1-x}\text{Li}_x\text{Sn}_2$  ( $x = 0.035$ ), crystallizes in the orthorhombic  $\text{LuNiSn}_2$  structure type. The asymmetric unit contains three Tm sites, six Sn sites, two Ni sites and one Ni/Li site [relative occupancies = 0.895 (8):0.185 (8)]. Site symmetries are  $m$  for all atoms. The 17-, 18- and 19-vertex distorted pseudo-Frank–Kasper polyhedra are typical for all Tm atoms. Four Sn atoms are enclosed in a 12-vertex deformed cubooctahedron, and another Sn atom is enclosed in a pentagonal prism with three added atoms. A tricapped trigonal prism is typical for a further Sn atom. The coordination number for all Ni atoms and Ni/Li statistical mixtures is 12 (fourcapped trigonal prism  $[\text{Ni/LiTm}_5\text{Sn}_5]$ ). Tm atoms form the base of a prism and Ni/Li atoms are at the centres of the side faces of an  $[\text{SnTm}_6\text{Ni/Li}_3]$  prism. These isolated prisms are implemented into three-dimensional-nets built out of Sn atoms. Electronic structure calculations using TB-LMTO-ASA suggest that the Tm and Ni/Li atoms form positively charged  $n[\text{TmNi/Li}]^{m+}$  polycations which compensate the negative charge of  $2n[\text{Sn}]^{m-}$  polyanions. Analysis of the interatomic distances and electronic structure calculations indicate the dominance of a metallic type of bonding.

## Related literature

For isotopic structures, see: Komarovskaya *et al.* (1983). For background of the study and related structures, see: Pavlyuk & Bodak (1992*a,b*); Pavlyuk *et al.* (1989*a,b*, 1991, 1993); Stetskiv *et al.* (2012, 2013). For electronic structure calculations, see: Andersen *et al.* (1986).

## Experimental

### Crystal data

|   |                                   |
|---|-----------------------------------|
| $\text{TmNi}_{0.965}\text{Li}_{0.035}\text{Sn}_2$ | $V = 1010.16$ (14) Å <sup>3</sup> |
| $M_r = 463.23$                                    | $Z = 12$                          |
| Orthorhombic, $Pnma$                              | Mo $K\alpha$ radiation            |
| $a = 16.0285$ (11) Å                              | $\mu = 45.77$ mm <sup>-1</sup>    |
| $b = 4.3862$ (4) Å                                | $T = 293$ K                       |
| $c = 14.3684$ (10) Å                              | $0.07 \times 0.03 \times 0.02$ mm |

### Data collection

|   |  |
|---|--|
| Oxford Diffraction Xcalibur3 CCD diffractometer                                     | 6737 measured reflections              |
| Absorption correction: analytical ( <i>CrysAlis RED</i> ; Oxford Diffraction, 2008) | 1304 independent reflections           |
| $T_{\min} = 0.213$ , $T_{\max} = 0.403$   | 1096 reflections with $I > 2\sigma(I)$ |
|   | $R_{\text{int}} = 0.034$               |

### Refinement

|                                 |   |
|---------------------------------|---|
| $R[F^2 > 2\sigma(F^2)] = 0.026$ | 76 parameters                                 |
| $wR(F^2) = 0.060$               | $\Delta\rho_{\max} = 2.07$ e Å <sup>-3</sup>  |
| $S = 1.18$                      | $\Delta\rho_{\min} = -2.13$ e Å <sup>-3</sup> |
| 1304 reflections                |   |

Data collection: *CrysAlis CCD* (Oxford Diffraction, 2008); cell refinement: *CrysAlis CCD*; data reduction: *CrysAlis RED* (Oxford Diffraction, 2008); program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *DIAMOND* (Brandenburg, 2006); software used to prepare material for publication: *SHELXL97*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: FF2120).

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## supplementary materials

*Acta Cryst.* (2013). E69, i76 [doi:10.1107/S1600536813027335]

**Thulium nickel/lithium distannide,  $\text{TmNi}_{1-x}\text{Li}_x\text{Sn}_2$  ( $x = 0.035$ )**

**Andriy Stetskiv, Ivan Tarasiuk, Renata Misztal and Volodymyr Pavlyuk**

**1. Comment**

The  $\text{RETSn}_2$  and  $\text{RET}_x\text{Sn}_2$  ( $x < 1$ ) type metallic compounds where RE is a rare-earth element (Gd—Lu) and T is a d-electron element crystallize in different orthorhombic crystal structures  $\text{LuNiSn}_2$  (space group  $Pnma$ ) and  $\text{CeNiSi}_2$ -type (space group  $Cmcm$ ) respectively. In the ternary  $\text{RELiSn}_2$  compounds lithium atoms occupy the same crystallographic position as the atoms of transition metal in the original  $\text{CeNiSi}_2$  structure type (Pavlyuk *et al.*, 1989a). Previous structural studies of the four-component alloys from  $\text{TbLiSn}_2$ — $\text{TbZnSn}_2$  sections indicate the existence of  $\text{TbLi}_{1-x}\text{Zn}_x\text{Sn}_2$  limited solid solution (Stetskiv *et al.*, 2012). X-ray single-crystal study showed that the  $\text{TbLi}_{1-x}\text{Zn}_x\text{Sn}_2$  solid solution was formed by the partial substitution of lithium atoms by zinc atoms in  $4c$  site. The ability of lithium atoms to partially substitute the atoms of transition metals was previously observed by us while studying solid solutions  $\text{RELiCu}_{2-x}\text{Si}_2$  and  $\text{RELiCu}_{2-x}\text{Ge}_2$  (Pavlyuk *et al.*, 1993). The ordered substitution of transition metals by lithium is observed for  $\text{Tm}_{2.22}\text{Co}_6\text{Sn}_{20}$  and  $\text{TmLi}_2\text{Co}_6\text{Sn}_{20}$  stannides (Stetskiv *et al.*, 2013). The ability of lithium atoms to occupy the same crystallographic position as the atoms of transition metal was observed previously while studying compounds  $\text{RELiGe}$  with the  $\text{ZrNiAl}$ -type (Pavlyuk *et al.*, 1991 and Pavlyuk & Bodak, 1992a),  $\text{RE}_3\text{Li}_2\text{Ge}_3$  with  $\text{Hf}_3\text{Ni}_2\text{Si}_3$ -type (Pavlyuk & Bodak, 1992b) and  $\text{Yb}_5\text{Li}_4\text{Ge}_4$  with  $\text{Nb}_5\text{Cu}_4\text{Si}_4$ -type (Pavlyuk *et al.*, 1989b).

The four-component phase  $\text{TmNi}_{1-x}\text{Li}_x\text{Sn}_2$  with low content of lithium from the  $\text{TmLiSn}_2$ — $\text{TmNiSn}_2$  section was detected by us during the systematic study of alloys of  $\text{Tm}$ — $\text{Ni}$ — $\text{Li}$ — $\text{Sn}$  system. Selected single-crystal data show that the title compound crystallizes with the orthorhombic space group  $Pnma$  as a  $\text{LuNiSn}_2$ -type (Komarovskaya *et al.*, 1983). The projection of the unit cell and coordination polyhedra of the atoms are shown in Fig. 1. The Tm atoms are enclosed in 17-, 18- and 19-vertex distorted pseudo Frank-Kasper polyhedra. The coordination polyhedron of Sn4, Sn7, Sn8 and Sn9 atoms is 12-vertex distorted cubooctahedron. The Sn5 is enclosed in pentagonal prism with three added atoms. The tricapped trigonal prism is typical for Sn6 atom. The environment of the Ni atoms and Ni/Li statistical mixture is a fourcapped trigonal prism and a coordination number equals 10 ( $\text{Tm}_5\text{Sn}_5$ ).

The distribution of nickel/lithium and thulium atoms in three-dimensional-nets built of Sn atoms is shown in Fig. 2. The thulium and nickel/lithium atoms form tricapped trigonal prism around Sn6. Thulium atoms form the base of prism and nickel/lithium atoms centre side faces of  $[\text{SnTm}_6\text{Ni/Li}_3]$  prism. These isolated prisms are implemented into three-dimensional-nets built of tin atoms. The data of electronic structure calculations using the TB-LMTO-ASA (Andersen *et al.*, 1986) suggest that thulium and nickel/lithium atoms form a positively charged  $n[\text{TmNi/Li}]^{m+}$  polycations which compensate the negative charge of  $2n[\text{Sn}]^{m-}$  polyanions (Fig. 3 A). Of course, this suggestion is based on the partial charges. All interatomic distances are values which correlate well with the atomic size; metallic type of bonding was indicated. A significant density of states (DOS) at the Fermi level (Fig. 3B) also indicates dominance of metallic bonding.

## 2. Experimental

Thulium, nickel, lithium and tin, all with a nominal purity more than 99.9 wt. %, were used as starting elements. First, the pieces of the pure metals with a stoichiometry  $\text{Tm}_{25}\text{Ni}_{20}\text{Li}_5\text{Sn}_{50}$  were pressed into pellet, enclosed in tantalum crucible and placed in a resistance furnace with a thermocouple controller. Heating rate from room temperature to 670 K was equal to 5 K per minute. At this temperature the alloy was kept over 2 d and then the temperature was increased from 670 to 1070 K over 1 h. Then, the alloy was annealed at this temperature for 8 h and slowly cooled down to room temperature. After the melting and annealing procedures, the total weight loss was less than 2%. Small good quality single-crystal of the title compound was isolated from the alloy.

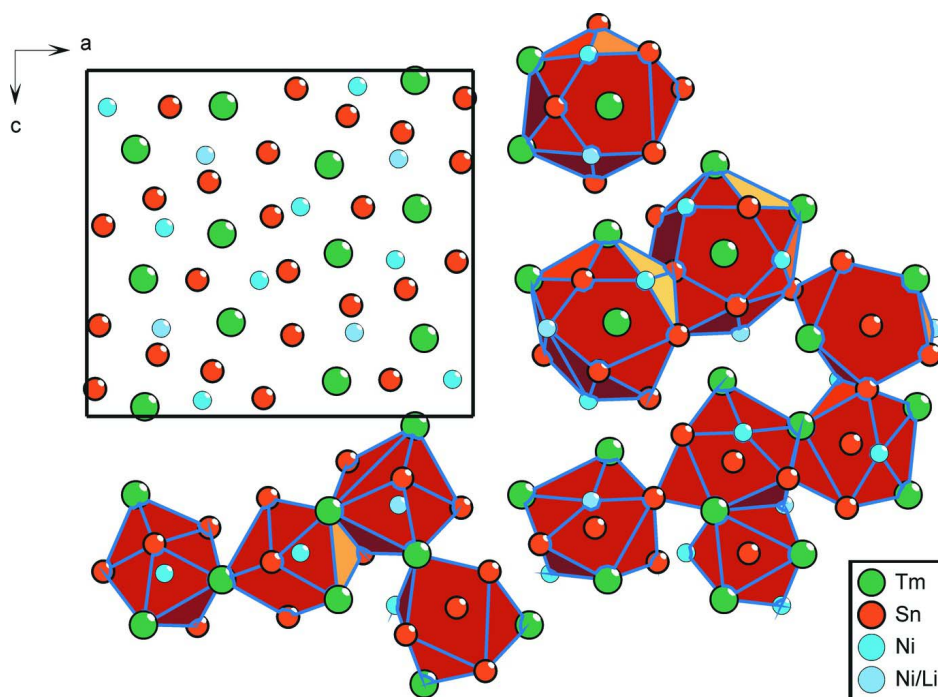
The synthesized alloy is practically single-phase. Therefore, in order to confirm the accuracy of the compositions, the density of the alloy was determined using the volumetric method. The measured density is  $9.08(5) \text{ Mg m}^{-3}$ , and these values differ by less than 1% from the densities calculated from the X-ray data. For the  $\text{TmNiSn}_2$  ternary phase density is  $9.19 \text{ Mg m}^{-3}$  (Komarovskaya *et al.*, 1983).

## 3. Refinement

The structure of the title phase was solved by direct methods after the analytical absorption correction. In the first stage of the refinement, the thermal displacement parameter of Ni12 atom was considerably different from those of other Ni sites, suggesting that this position is partially occupied by the lithium atom. In the final refinement cycles all atoms were successfully refined with anisotropic displacement parameters.

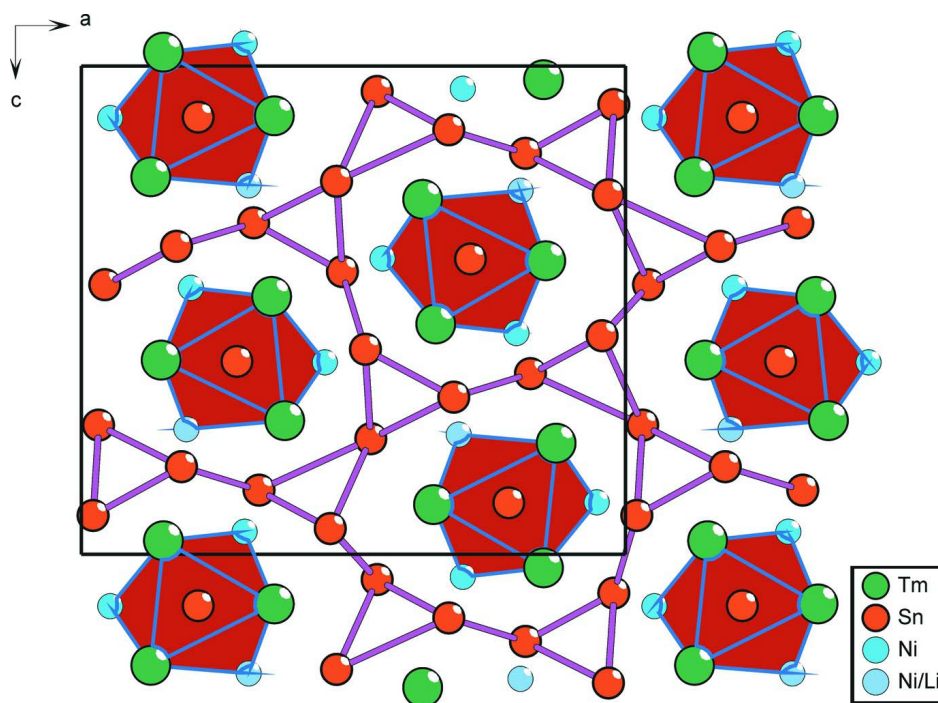
## Computing details

Data collection: *CrysAlis CCD* (Oxford Diffraction, 2008); cell refinement: *CrysAlis CCD* (Oxford Diffraction, 2008); data reduction: *CrysAlis RED* (Oxford Diffraction, 2008); program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *DIAMOND* (Brandenburg, 2006); software used to prepare material for publication: *SHELXL97* (Sheldrick, 2008).



**Figure 1**

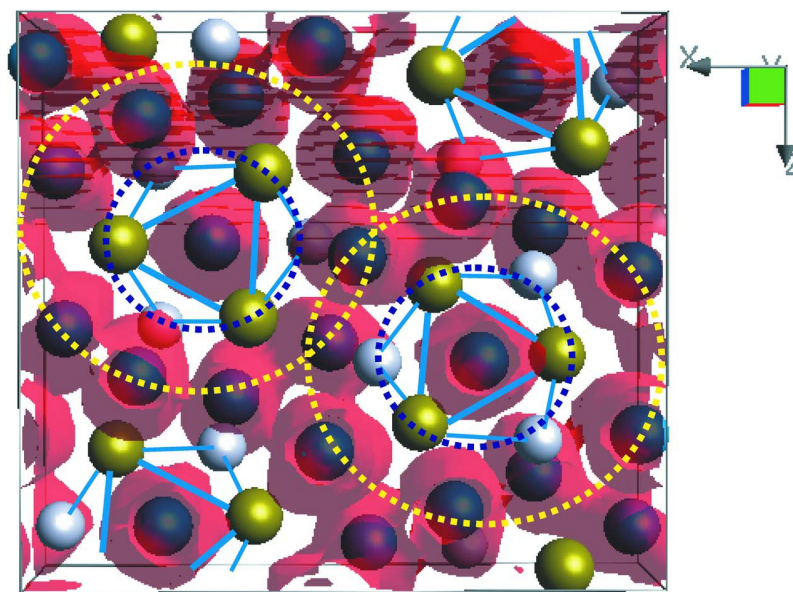
The projection of the unit cell and coordination polyhedra of the atoms.



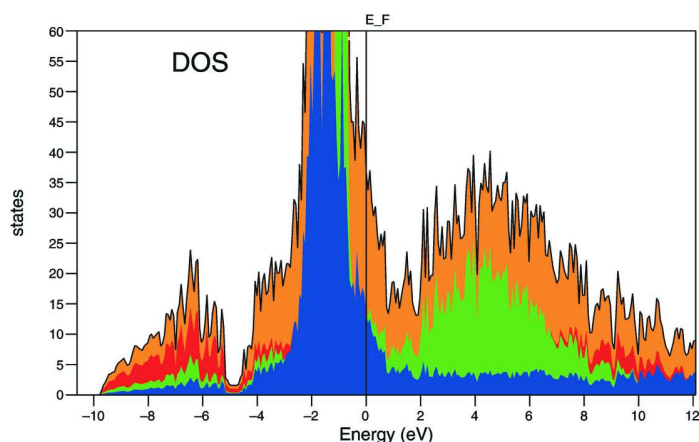
**Figure 2**

The distribution of thulium and nickel/lithium atoms in three-dimensional-nets built of the Sn atoms.

A



B



**Figure 3**

(A) Isosurfaces of electron localization function (ELF) around the atoms, positively charged  $n[\text{TmNi/Li}]^{m+}$  polycations marked by the violet dotted line and the negatively charged  $2n[\text{Sn}]^{m-}$  polyanions marked by the yellow dotted line. (B) Total and partial DOS.

### Thulium nickel/lithium distannide

#### Crystal data

$\text{TmNi}_{0.965}\text{Li}_{0.035}\text{Sn}_2$   
 $M_r = 463.23$   
 Orthorhombic,  $Pnma$   
 Hall symbol:  $-P\ 2ac\ 2n$   
 $a = 16.0285\ (11)\ \text{\AA}$   
 $b = 4.3862\ (4)\ \text{\AA}$   
 $c = 14.3684\ (10)\ \text{\AA}$

$V = 1010.16\ (14)\ \text{\AA}^3$   
 $Z = 12$   
 $F(000) = 2353.5$   
 $D_x = 9.138\ \text{Mg m}^{-3}$   
 Mo  $K\alpha$  radiation,  $\lambda = 0.71073\ \text{\AA}$   
 Cell parameters from 1304 reflections  
 $\theta = 3.8\text{--}27.5^\circ$

$\mu = 45.77 \text{ mm}^{-1}$   
 $T = 293 \text{ K}$

Prism, metallic dark gray  
 $0.07 \times 0.03 \times 0.02 \text{ mm}$

#### Data collection

Oxford Diffraction Xcalibur3 CCD  
 diffractometer  
 Radiation source: fine-focus sealed tube  
 Graphite monochromator  
 Detector resolution: 0 pixels  $\text{mm}^{-1}$   
 $\omega$  scans  
 Absorption correction: analytical  
 (CrysAlis RED; Oxford Diffraction, 2008)  
 $T_{\min} = 0.213$ ,  $T_{\max} = 0.403$

6737 measured reflections  
 1304 independent reflections  
 1096 reflections with  $I > 2\sigma(I)$   
 $R_{\text{int}} = 0.034$   
 $\theta_{\max} = 27.5^\circ$ ,  $\theta_{\min} = 3.8^\circ$   
 $h = -20 \rightarrow 20$   
 $k = -3 \rightarrow 5$   
 $l = -18 \rightarrow 18$

#### Refinement

Refinement on  $F^2$   
 Least-squares matrix: full  
 $R[F^2 > 2\sigma(F^2)] = 0.026$   
 $wR(F^2) = 0.060$   
 $S = 1.18$   
 1304 reflections  
 76 parameters  
 0 restraints  
 Primary atom site location: structure-invariant  
 direct methods

Secondary atom site location: difference Fourier  
 map  
 $w = 1/[\sigma^2(F_o^2) + (0.023P)^2 + 11.3465P]$   
 where  $P = (F_o^2 + 2F_c^2)/3$   
 $(\Delta/\sigma)_{\max} = 0.006$   
 $\Delta\rho_{\max} = 2.07 \text{ e } \text{\AA}^{-3}$   
 $\Delta\rho_{\min} = -2.13 \text{ e } \text{\AA}^{-3}$   
 Extinction correction: SHELXL97 (Sheldrick,  
 2008),  $F_c^* = kF_c[1 + 0.001x F_c^2 \lambda^3 / \sin(2\theta)]^{-1/4}$   
 Extinction coefficient: 0.00030 (3)

#### Special details

**Geometry.** All e.s.d.'s (except the e.s.d. in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell e.s.d.'s are taken into account individually in the estimation of e.s.d.'s in distances, angles and torsion angles; correlations between e.s.d.'s in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell e.s.d.'s is used for estimating e.s.d.'s involving l.s. planes.

**Refinement.** Refinement of  $F^2$  against ALL reflections. The weighted  $R$ -factor  $wR$  and goodness of fit  $S$  are based on  $F^2$ , conventional  $R$ -factors  $R$  are based on  $F$ , with  $F$  set to zero for negative  $F^2$ . The threshold expression of  $F^2 > \sigma(F^2)$  is used only for calculating  $R$ -factors(gt) etc. and is not relevant to the choice of reflections for refinement.  $R$ -factors based on  $F^2$  are statistically about twice as large as those based on  $F$ , and  $R$ -factors based on ALL data will be even larger.

#### Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters ( $\text{\AA}^2$ )

|      | <i>x</i>     | <i>y</i> | <i>z</i>      | $U_{\text{iso}}^*/U_{\text{eq}}$ | Occ. (<1) |
|------|--------------|----------|---------------|----------------------------------|-----------|
| Tm1  | 0.35386 (4)  | 0.2500   | 0.10177 (4)   | 0.01166 (15)                     |           |
| Tm2  | 0.15061 (4)  | 0.2500   | -0.02797 (4)  | 0.01120 (15)                     |           |
| Tm3  | 0.12704 (4)  | 0.2500   | 0.22713 (4)   | 0.01269 (15)                     |           |
| Sn4  | 0.02119 (5)  | -0.2500  | -0.07931 (6)  | 0.0105 (2)                       |           |
| Sn5  | 0.46864 (6)  | -0.2500  | 0.23607 (7)   | 0.0158 (2)                       |           |
| Sn6  | 0.21452 (6)  | -0.2500  | 0.10507 (6)   | 0.0129 (2)                       |           |
| Sn7  | 0.32559 (6)  | 0.2500   | -0.13071 (6)  | 0.0118 (2)                       |           |
| Sn8  | 0.31632 (6)  | 0.2500   | 0.32114 (7)   | 0.0157 (2)                       |           |
| Sn9  | 0.45722 (6)  | -0.2500  | -0.05229 (7)  | 0.0154 (2)                       |           |
| Ni10 | 0.29945 (11) | -0.2500  | -0.04622 (13) | 0.0133 (4)                       |           |
| Ni11 | 0.05291 (10) | -0.2500  | 0.10639 (12)  | 0.0122 (4)                       |           |
| Ni12 | 0.30709 (12) | -0.2500  | 0.24440 (14)  | 0.0162 (7)                       | 0.895 (8) |
| Li12 | 0.30709 (12) | -0.2500  | 0.24440 (14)  | 0.0162 (7)                       | 0.105 (8) |

*Atomic displacement parameters ( $\text{\AA}^2$ )*

|      | $U^{11}$    | $U^{22}$    | $U^{33}$    | $U^{12}$ | $U^{13}$    | $U^{23}$ |
|------|-------------|-------------|-------------|----------|-------------|----------|
| Tm1  | 0.0109 (3)  | 0.0140 (3)  | 0.0100 (3)  | 0.000    | 0.0005 (2)  | 0.000    |
| Tm2  | 0.0107 (3)  | 0.0124 (3)  | 0.0105 (3)  | 0.000    | 0.0011 (2)  | 0.000    |
| Tm3  | 0.0157 (3)  | 0.0136 (3)  | 0.0087 (3)  | 0.000    | −0.0028 (2) | 0.000    |
| Sn4  | 0.0092 (4)  | 0.0106 (4)  | 0.0117 (4)  | 0.000    | 0.0002 (3)  | 0.000    |
| Sn5  | 0.0162 (5)  | 0.0174 (4)  | 0.0138 (5)  | 0.000    | −0.0035 (4) | 0.000    |
| Sn6  | 0.0117 (5)  | 0.0124 (4)  | 0.0145 (5)  | 0.000    | 0.0009 (3)  | 0.000    |
| Sn7  | 0.0140 (5)  | 0.0106 (4)  | 0.0107 (5)  | 0.000    | 0.0014 (3)  | 0.000    |
| Sn8  | 0.0114 (5)  | 0.0231 (5)  | 0.0127 (5)  | 0.000    | −0.0001 (3) | 0.000    |
| Sn9  | 0.0087 (5)  | 0.0174 (5)  | 0.0201 (5)  | 0.000    | −0.0015 (4) | 0.000    |
| Ni10 | 0.0117 (9)  | 0.0143 (8)  | 0.0138 (9)  | 0.000    | −0.0009 (7) | 0.000    |
| Ni11 | 0.0116 (8)  | 0.0124 (8)  | 0.0127 (9)  | 0.000    | −0.0004 (6) | 0.000    |
| Ni12 | 0.0220 (12) | 0.0148 (11) | 0.0117 (11) | 0.000    | −0.0044 (8) | 0.000    |
| Li12 | 0.0220 (12) | 0.0148 (11) | 0.0117 (11) | 0.000    | −0.0044 (8) | 0.000    |

*Geometric parameters ( $\text{\AA}$ ,  $^\circ$ )*

|                        |             |                         |             |
|------------------------|-------------|-------------------------|-------------|
| Tm1—Li12 <sup>i</sup>  | 3.0938 (15) | Sn5—Tm1 <sup>xi</sup>   | 3.4522 (9)  |
| Tm1—Ni12 <sup>i</sup>  | 3.0938 (15) | Sn6—Ni12                | 2.492 (2)   |
| Tm1—Ni12               | 3.0938 (15) | Sn6—Ni10                | 2.565 (2)   |
| Tm1—Sn9 <sup>ii</sup>  | 3.1104 (11) | Sn6—Ni11                | 2.5904 (19) |
| Tm1—Sn6                | 3.1306 (8)  | Sn6—Tm2 <sup>xi</sup>   | 3.0844 (8)  |
| Tm1—Sn6 <sup>i</sup>   | 3.1306 (8)  | Sn6—Tm1 <sup>xi</sup>   | 3.1306 (8)  |
| Tm1—Ni10               | 3.1768 (14) | Sn6—Tm3 <sup>xi</sup>   | 3.1387 (8)  |
| Tm1—Ni10 <sup>i</sup>  | 3.1768 (14) | Sn7—Ni10 <sup>i</sup>   | 2.5415 (10) |
| Tm1—Sn8                | 3.2089 (11) | Sn7—Ni10                | 2.5415 (10) |
| Tm1—Sn7                | 3.3711 (11) | Sn7—Li12 <sup>iii</sup> | 2.783 (2)   |
| Tm1—Sn5 <sup>i</sup>   | 3.4522 (9)  | Sn7—Ni12 <sup>iii</sup> | 2.783 (2)   |
| Tm2—Sn6 <sup>i</sup>   | 3.0844 (8)  | Sn7—Tm3 <sup>iii</sup>  | 3.0916 (8)  |
| Tm2—Sn6                | 3.0844 (8)  | Sn7—Tm3 <sup>iv</sup>   | 3.0916 (8)  |
| Tm2—Sn4                | 3.1076 (8)  | Sn7—Sn8 <sup>iii</sup>  | 3.2345 (9)  |
| Tm2—Sn4 <sup>i</sup>   | 3.1076 (8)  | Sn7—Sn8 <sup>iv</sup>   | 3.2345 (9)  |
| Tm2—Sn8 <sup>iii</sup> | 3.1290 (8)  | Sn7—Sn9 <sup>i</sup>    | 3.2451 (10) |
| Tm2—Sn8 <sup>iv</sup>  | 3.1290 (8)  | Sn7—Sn9                 | 3.2451 (10) |
| Tm2—Sn4 <sup>v</sup>   | 3.1557 (11) | Sn8—Ni12                | 2.4591 (10) |
| Tm2—Sn7                | 3.1695 (11) | Sn8—Li12 <sup>i</sup>   | 2.4591 (10) |
| Tm2—Ni10 <sup>i</sup>  | 3.2512 (13) | Sn8—Ni12 <sup>i</sup>   | 2.4591 (10) |
| Tm2—Ni10               | 3.2512 (13) | Sn8—Ni10 <sup>vii</sup> | 2.660 (2)   |
| Tm2—Ni11 <sup>i</sup>  | 3.3150 (13) | Sn8—Sn4 <sup>vii</sup>  | 2.9714 (13) |
| Tm2—Ni11               | 3.3150 (13) | Sn8—Tm2 <sup>vi</sup>   | 3.1290 (8)  |
| Tm3—Ni11               | 3.0383 (13) | Sn8—Tm2 <sup>vii</sup>  | 3.1290 (8)  |
| Tm3—Ni11 <sup>i</sup>  | 3.0383 (13) | Sn8—Sn7 <sup>vii</sup>  | 3.2345 (9)  |
| Tm3—Sn7 <sup>vi</sup>  | 3.0916 (8)  | Sn8—Sn7 <sup>vi</sup>   | 3.2345 (9)  |
| Tm3—Sn7 <sup>vii</sup> | 3.0916 (8)  | Sn9—Ni10                | 2.5303 (19) |
| Tm3—Sn6                | 3.1387 (8)  | Sn9—Sn9 <sup>ii</sup>   | 2.9914 (13) |
| Tm3—Sn6 <sup>i</sup>   | 3.1387 (8)  | Sn9—Sn9 <sup>xiv</sup>  | 2.9914 (13) |
| Tm3—Sn4 <sup>v</sup>   | 3.1868 (10) | Sn9—Tm1 <sup>ii</sup>   | 3.1104 (11) |
| Tm3—Sn8                | 3.3210 (11) | Sn9—Sn7 <sup>xi</sup>   | 3.2451 (10) |

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| Tm3—Sn5 <sup>viii</sup>                  | 3.3963 (8)   | Sn9—Tm3 <sup>iii</sup>                       | 3.4450 (12) |
| Tm3—Sn5 <sup>ix</sup>                    | 3.3963 (8)   | Sn9—Tm1 <sup>xi</sup>                        | 3.5291 (9)  |
| Tm3—Sn9 <sup>vii</sup>                   | 3.4450 (12)  | Ni10—Sn7 <sup>xi</sup>                       | 2.5415 (10) |
| Tm3—Ni10 <sup>vii</sup>                  | 3.4631 (19)  | Ni10—Sn8 <sup>iii</sup>                      | 2.660 (2)   |
| Sn4—Ni11 <sup>x</sup>                    | 2.5242 (9)   | Ni10—Tm1 <sup>xi</sup>                       | 3.1768 (14) |
| Sn4—Ni11 <sup>v</sup>                    | 2.5242 (9)   | Ni10—Tm2 <sup>xi</sup>                       | 3.2512 (13) |
| Sn4—Ni11                                 | 2.7163 (19)  | Ni10—Tm3 <sup>iii</sup>                      | 3.4631 (19) |
| Sn4—Sn8 <sup>iii</sup>                   | 2.9714 (13)  | Ni11—Sn4 <sup>x</sup>                        | 2.5242 (9)  |
| Sn4—Tm2 <sup>xi</sup>                    | 3.1076 (8)   | Ni11—Sn4 <sup>v</sup>                        | 2.5242 (9)  |
| Sn4—Tm2 <sup>v</sup>                     | 3.1557 (11)  | Ni11—Sn5 <sup>viii</sup>                     | 2.636 (2)   |
| Sn4—Tm3 <sup>v</sup>                     | 3.1868 (10)  | Ni11—Tm3 <sup>xi</sup>                       | 3.0383 (13) |
| Sn4—Sn4 <sup>v</sup>                     | 3.2350 (13)  | Ni11—Tm2 <sup>xi</sup>                       | 3.3150 (13) |
| Sn4—Sn4 <sup>x</sup>                     | 3.2350 (13)  | Ni11—Tm2 <sup>v</sup>                        | 3.4512 (17) |
| Sn5—Ni12                                 | 2.592 (2)    | Ni12—Sn8 <sup>xi</sup>                       | 2.4591 (10) |
| Sn5—Ni11 <sup>xii</sup>                  | 2.636 (2)    | Ni12—Sn7 <sup>vii</sup>                      | 2.783 (2)   |
| Sn5—Tm3 <sup>xii</sup>                   | 3.3963 (9)   | Ni12—Tm1 <sup>xi</sup>                       | 3.0938 (15) |
| Sn5—Tm3 <sup>xiii</sup>                  | 3.3963 (8)   | Ni12—Tm2 <sup>vii</sup>                      | 3.340 (2)   |
| Li12 <sup>i</sup> —Tm1—Ni12 <sup>i</sup> | 0.00 (9)     | Tm2—Sn6—Tm3                                  | 72.611 (17) |
| Li12 <sup>i</sup> —Tm1—Ni12              | 90.29 (6)    | Tm1—Sn6—Tm3                                  | 80.659 (16) |
| Ni12 <sup>i</sup> —Tm1—Ni12              | 90.29 (6)    | Tm1 <sup>xi</sup> —Sn6—Tm3                   | 144.75 (4)  |
| Li12 <sup>i</sup> —Tm1—Sn9 <sup>ii</sup> | 112.79 (4)   | Tm3 <sup>xi</sup> —Sn6—Tm3                   | 88.65 (3)   |
| Ni12 <sup>i</sup> —Tm1—Sn9 <sup>ii</sup> | 112.79 (4)   | Ni10 <sup>i</sup> —Sn7—Ni10                  | 119.29 (8)  |
| Ni12—Tm1—Sn9 <sup>ii</sup>               | 112.79 (4)   | Ni10 <sup>i</sup> —Sn7—Li12 <sup>iii</sup>   | 100.49 (5)  |
| Li12 <sup>i</sup> —Tm1—Sn6               | 108.28 (4)   | Ni10—Sn7—Li12 <sup>iii</sup>                 | 100.49 (5)  |
| Ni12 <sup>i</sup> —Tm1—Sn6               | 108.28 (4)   | Ni10 <sup>i</sup> —Sn7—Ni12 <sup>iii</sup>   | 100.49 (5)  |
| Ni12—Tm1—Sn6                             | 47.19 (4)    | Ni10—Sn7—Ni12 <sup>iii</sup>                 | 100.49 (5)  |
| Sn9 <sup>ii</sup> —Tm1—Sn6               | 134.268 (15) | Li12 <sup>iii</sup> —Sn7—Ni12 <sup>iii</sup> | 0.00 (8)    |
| Li12 <sup>i</sup> —Tm1—Sn6 <sup>i</sup>  | 47.19 (4)    | Ni10 <sup>i</sup> —Sn7—Tm3 <sup>iii</sup>    | 165.51 (5)  |
| Ni12 <sup>i</sup> —Tm1—Sn6 <sup>i</sup>  | 47.19 (4)    | Ni10—Sn7—Tm3 <sup>iii</sup>                  | 75.16 (4)   |
| Ni12—Tm1—Sn6 <sup>i</sup>                | 108.28 (4)   | Li12 <sup>iii</sup> —Sn7—Tm3 <sup>iii</sup>  | 76.21 (4)   |
| Sn9 <sup>ii</sup> —Tm1—Sn6 <sup>i</sup>  | 134.268 (15) | Ni12 <sup>iii</sup> —Sn7—Tm3 <sup>iii</sup>  | 76.21 (4)   |
| Sn6—Tm1—Sn6 <sup>i</sup>                 | 88.94 (3)    | Ni10 <sup>i</sup> —Sn7—Tm3 <sup>iv</sup>     | 75.16 (4)   |
| Li12 <sup>i</sup> —Tm1—Ni10              | 150.02 (5)   | Ni10—Sn7—Tm3 <sup>iv</sup>                   | 165.51 (5)  |
| Ni12 <sup>i</sup> —Tm1—Ni10              | 150.02 (5)   | Li12 <sup>iii</sup> —Sn7—Tm3 <sup>iv</sup>   | 76.21 (4)   |
| Ni12—Tm1—Ni10                            | 83.54 (4)    | Ni12 <sup>iii</sup> —Sn7—Tm3 <sup>iv</sup>   | 76.21 (4)   |
| Sn9 <sup>ii</sup> —Tm1—Ni10              | 96.56 (4)    | Tm3 <sup>iii</sup> —Sn7—Tm3 <sup>iv</sup>    | 90.37 (3)   |
| Sn6—Tm1—Ni10                             | 47.98 (4)    | Ni10 <sup>i</sup> —Sn7—Tm2                   | 68.39 (4)   |
| Sn6 <sup>i</sup> —Tm1—Ni10               | 107.33 (3)   | Ni10—Sn7—Tm2                                 | 68.39 (4)   |
| Li12 <sup>i</sup> —Tm1—Ni10 <sup>i</sup> | 83.54 (4)    | Li12 <sup>iii</sup> —Sn7—Tm2                 | 67.91 (5)   |
| Ni12 <sup>i</sup> —Tm1—Ni10 <sup>i</sup> | 83.54 (4)    | Ni12 <sup>iii</sup> —Sn7—Tm2                 | 67.91 (5)   |
| Ni12—Tm1—Ni10 <sup>i</sup>               | 150.02 (5)   | Tm3 <sup>iii</sup> —Sn7—Tm2                  | 121.67 (2)  |
| Sn9 <sup>ii</sup> —Tm1—Ni10 <sup>i</sup> | 96.56 (4)    | Tm3 <sup>iv</sup> —Sn7—Tm2                   | 121.67 (2)  |
| Sn6—Tm1—Ni10 <sup>i</sup>                | 107.33 (3)   | Ni10 <sup>i</sup> —Sn7—Sn8 <sup>iii</sup>    | 124.84 (5)  |
| Sn6 <sup>i</sup> —Tm1—Ni10 <sup>i</sup>  | 47.98 (4)    | Ni10—Sn7—Sn8 <sup>iii</sup>                  | 53.21 (4)   |
| Ni10—Tm1—Ni10 <sup>i</sup>               | 87.31 (5)    | Li12 <sup>iii</sup> —Sn7—Sn8 <sup>iii</sup>  | 47.52 (2)   |
| Li12 <sup>i</sup> —Tm1—Sn8               | 45.89 (3)    | Ni12 <sup>iii</sup> —Sn7—Sn8 <sup>iii</sup>  | 47.52 (2)   |
| Ni12 <sup>i</sup> —Tm1—Sn8               | 45.89 (3)    | Tm3 <sup>iii</sup> —Sn7—Sn8 <sup>iii</sup>   | 63.28 (2)   |
| Ni12—Tm1—Sn8                             | 45.89 (3)    | Tm3 <sup>iv</sup> —Sn7—Sn8 <sup>iii</sup>    | 120.82 (3)  |



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| Sn9 <sup>ii</sup> —Tm1—Sn8                | 114.02 (3)  | Tm2—Sn7—Sn8 <sup>iii</sup>                  | 58.49 (2)   |
| Sn6—Tm1—Sn8                               | 81.45 (2)   | Ni10 <sup>i</sup> —Sn7—Sn8 <sup>iv</sup>    | 53.21 (4)   |
| Sn6 <sup>i</sup> —Tm1—Sn8                 | 81.45 (2)   | Ni10—Sn7—Sn8 <sup>iv</sup>                  | 124.84 (5)  |
| Ni10—Tm1—Sn8                              | 127.30 (3)  | Li12 <sup>iii</sup> —Sn7—Sn8 <sup>iv</sup>  | 47.52 (2)   |
| Ni10 <sup>i</sup> —Tm1—Sn8                | 127.30 (3)  | Ni12 <sup>iii</sup> —Sn7—Sn8 <sup>iv</sup>  | 47.52 (2)   |
| Li12 <sup>i</sup> —Tm1—Sn7                | 128.59 (3)  | Tm3 <sup>iii</sup> —Sn7—Sn8 <sup>iv</sup>   | 120.82 (3)  |
| Ni12 <sup>i</sup> —Tm1—Sn7                | 128.59 (3)  | Tm3 <sup>iv</sup> —Sn7—Sn8 <sup>iv</sup>    | 63.28 (2)   |
| Ni12—Tm1—Sn7                              | 128.59 (3)  | Tm2—Sn7—Sn8 <sup>iv</sup>                   | 58.49 (2)   |
| Sn9 <sup>ii</sup> —Tm1—Sn7                | 84.51 (3)   | Sn8 <sup>iii</sup> —Sn7—Sn8 <sup>iv</sup>   | 85.38 (3)   |
| Sn6—Tm1—Sn7                               | 85.36 (2)   | Ni10 <sup>i</sup> —Sn7—Sn9 <sup>i</sup>     | 50.07 (4)   |
| Sn6 <sup>i</sup> —Tm1—Sn7                 | 85.36 (2)   | Ni10—Sn7—Sn9 <sup>i</sup>                   | 121.64 (5)  |
| Ni10—Tm1—Sn7                              | 45.56 (3)   | Li12 <sup>iii</sup> —Sn7—Sn9 <sup>i</sup>   | 136.12 (2)  |
| Ni10 <sup>i</sup> —Tm1—Sn7                | 45.56 (3)   | Ni12 <sup>iii</sup> —Sn7—Sn9 <sup>i</sup>   | 136.12 (2)  |
| Sn8—Tm1—Sn7                               | 161.47 (3)  | Tm3 <sup>iii</sup> —Sn7—Sn9 <sup>i</sup>    | 123.31 (3)  |
| Li12 <sup>i</sup> —Tm1—Sn5 <sup>i</sup>   | 46.26 (4)   | Tm3 <sup>iv</sup> —Sn7—Sn9 <sup>i</sup>     | 65.81 (2)   |
| Ni12 <sup>i</sup> —Tm1—Sn5 <sup>i</sup>   | 46.26 (4)   | Tm2—Sn7—Sn9 <sup>i</sup>                    | 114.43 (3)  |
| Ni12—Tm1—Sn5 <sup>i</sup>                 | 102.08 (4)  | Sn8 <sup>iii</sup> —Sn7—Sn9 <sup>i</sup>    | 171.77 (4)  |
| Sn9 <sup>ii</sup> —Tm1—Sn5 <sup>i</sup>   | 66.98 (2)   | Sn8 <sup>iv</sup> —Sn7—Sn9 <sup>i</sup>     | 94.201 (17) |
| Sn6—Tm1—Sn5 <sup>i</sup>                  | 144.76 (3)  | Ni10 <sup>i</sup> —Sn7—Sn9                  | 121.64 (5)  |
| Sn6 <sup>i</sup> —Tm1—Sn5 <sup>i</sup>    | 85.797 (19) | Ni10—Sn7—Sn9                                | 50.07 (4)   |
| Ni10—Tm1—Sn5 <sup>i</sup>                 | 163.54 (4)  | Li12 <sup>iii</sup> —Sn7—Sn9                | 136.12 (2)  |
| Ni10 <sup>i</sup> —Tm1—Sn5 <sup>i</sup>   | 94.70 (3)   | Ni12 <sup>iii</sup> —Sn7—Sn9                | 136.12 (2)  |
| Sn8—Tm1—Sn5 <sup>i</sup>                  | 63.31 (2)   | Tm3 <sup>iii</sup> —Sn7—Sn9                 | 65.81 (2)   |
| Sn7—Tm1—Sn5 <sup>i</sup>                  | 128.72 (2)  | Tm3 <sup>iv</sup> —Sn7—Sn9                  | 123.31 (3)  |
| Sn6 <sup>i</sup> —Tm2—Sn6                 | 90.64 (3)   | Tm2—Sn7—Sn9                                 | 114.43 (3)  |
| Sn6 <sup>i</sup> —Tm2—Sn4                 | 150.53 (3)  | Sn8 <sup>iii</sup> —Sn7—Sn9                 | 94.201 (17) |
| Sn6—Tm2—Sn4                               | 82.359 (19) | Sn8 <sup>iv</sup> —Sn7—Sn9                  | 171.77 (4)  |
| Sn6 <sup>i</sup> —Tm2—Sn4 <sup>i</sup>    | 82.359 (19) | Sn9 <sup>i</sup> —Sn7—Sn9                   | 85.04 (3)   |
| Sn6—Tm2—Sn4 <sup>i</sup>                  | 150.53 (3)  | Ni10 <sup>i</sup> —Sn7—Tm1                  | 63.18 (4)   |
| Sn4—Tm2—Sn4 <sup>i</sup>                  | 89.78 (3)   | Ni10—Sn7—Tm1                                | 63.18 (4)   |
| Sn6 <sup>i</sup> —Tm2—Sn8 <sup>iii</sup>  | 150.63 (3)  | Li12 <sup>iii</sup> —Sn7—Tm1                | 137.88 (5)  |
| Sn6—Tm2—Sn8 <sup>iii</sup>                | 82.81 (2)   | Ni12 <sup>iii</sup> —Sn7—Tm1                | 137.88 (5)  |
| Sn4—Tm2—Sn8 <sup>iii</sup>                | 56.91 (2)   | Tm3 <sup>iii</sup> —Sn7—Tm1                 | 128.44 (2)  |
| Sn4 <sup>i</sup> —Tm2—Sn8 <sup>iii</sup>  | 116.31 (3)  | Tm3 <sup>iv</sup> —Sn7—Tm1                  | 128.44 (2)  |
| Sn6 <sup>i</sup> —Tm2—Sn8 <sup>iv</sup>   | 82.81 (2)   | Tm2—Sn7—Tm1                                 | 69.97 (2)   |
| Sn6—Tm2—Sn8 <sup>iv</sup>                 | 150.63 (3)  | Sn8 <sup>iii</sup> —Sn7—Tm1                 | 107.85 (3)  |
| Sn4—Tm2—Sn8 <sup>iv</sup>                 | 116.31 (3)  | Sn8 <sup>iv</sup> —Sn7—Tm1                  | 107.85 (3)  |
| Sn4 <sup>i</sup> —Tm2—Sn8 <sup>iv</sup>   | 56.91 (2)   | Sn9 <sup>i</sup> —Sn7—Tm1                   | 64.44 (2)   |
| Sn8 <sup>iii</sup> —Tm2—Sn8 <sup>iv</sup> | 89.00 (3)   | Sn9—Sn7—Tm1                                 | 64.44 (2)   |
| Sn6 <sup>i</sup> —Tm2—Sn4 <sup>v</sup>    | 89.26 (2)   | Ni12—Sn8—Li12 <sup>i</sup>                  | 126.20 (9)  |
| Sn6—Tm2—Sn4 <sup>v</sup>                  | 89.26 (2)   | Ni12—Sn8—Ni12 <sup>i</sup>                  | 126.20 (9)  |
| Sn4—Tm2—Sn4 <sup>v</sup>                  | 62.19 (2)   | Li12 <sup>i</sup> —Sn8—Ni12 <sup>i</sup>    | 0.00 (12)   |
| Sn4 <sup>i</sup> —Tm2—Sn4 <sup>v</sup>    | 62.19 (2)   | Ni12—Sn8—Ni10 <sup>vii</sup>                | 106.22 (5)  |
| Sn8 <sup>iii</sup> —Tm2—Sn4 <sup>v</sup>  | 119.10 (2)  | Li12 <sup>i</sup> —Sn8—Ni10 <sup>vii</sup>  | 106.22 (5)  |
| Sn8 <sup>iv</sup> —Tm2—Sn4 <sup>v</sup>   | 119.10 (2)  | Ni12 <sup>i</sup> —Sn8—Ni10 <sup>vii</sup>  | 106.22 (5)  |
| Sn6 <sup>i</sup> —Tm2—Sn7                 | 89.70 (2)   | Ni12—Sn8—Sn4 <sup>vii</sup>                 | 105.58 (5)  |
| Sn6—Tm2—Sn7                               | 89.70 (2)   | Li12 <sup>i</sup> —Sn8—Sn4 <sup>vii</sup>   | 105.58 (5)  |
| Sn4—Tm2—Sn7                               | 118.70 (2)  | Ni12 <sup>i</sup> —Sn8—Sn4 <sup>vii</sup>   | 105.58 (5)  |
| Sn4 <sup>i</sup> —Tm2—Sn7                 | 118.70 (2)  | Ni10 <sup>vii</sup> —Sn8—Sn4 <sup>vii</sup> | 105.46 (5)  |

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| Sn8 <sup>iii</sup> —Tm2—Sn7               | 61.80 (2)  | Ni12—Sn8—Tm2 <sup>vi</sup>                  | 161.07 (5) |
| Sn8 <sup>iv</sup> —Tm2—Sn7                | 61.80 (2)  | Li12 <sup>i</sup> —Sn8—Tm2 <sup>vi</sup>    | 72.29 (4)  |
| Sn4 <sup>v</sup> —Tm2—Sn7                 | 178.52 (3) | Ni12 <sup>i</sup> —Sn8—Tm2 <sup>vi</sup>    | 72.29 (4)  |
| Sn6 <sup>i</sup> —Tm2—Ni10 <sup>i</sup>   | 47.67 (3)  | Ni10 <sup>vii</sup> —Sn8—Tm2 <sup>vi</sup>  | 67.78 (3)  |
| Sn6—Tm2—Ni10 <sup>i</sup>                 | 106.61 (3) | Sn4 <sup>vii</sup> —Sn8—Tm2 <sup>vi</sup>   | 61.18 (2)  |
| Sn4—Tm2—Ni10 <sup>i</sup>                 | 161.22 (4) | Ni12—Sn8—Tm2 <sup>vii</sup>                 | 72.29 (4)  |
| Sn4 <sup>i</sup> —Tm2—Ni10 <sup>i</sup>   | 89.69 (3)  | Li12 <sup>i</sup> —Sn8—Tm2 <sup>vii</sup>   | 161.07 (5) |
| Sn8 <sup>iii</sup> —Tm2—Ni10 <sup>i</sup> | 107.01 (3) | Ni12 <sup>i</sup> —Sn8—Tm2 <sup>vii</sup>   | 161.07 (5) |
| Sn8 <sup>iv</sup> —Tm2—Ni10 <sup>i</sup>  | 49.23 (3)  | Ni10 <sup>vii</sup> —Sn8—Tm2 <sup>vii</sup> | 67.78 (3)  |
| Sn4 <sup>v</sup> —Tm2—Ni10 <sup>i</sup>   | 132.82 (3) | Sn4 <sup>vii</sup> —Sn8—Tm2 <sup>vii</sup>  | 61.18 (2)  |
| Sn7—Tm2—Ni10 <sup>i</sup>                 | 46.61 (3)  | Tm2 <sup>vi</sup> —Sn8—Tm2 <sup>vii</sup>   | 89.00 (3)  |
| Sn6 <sup>i</sup> —Tm2—Ni10                | 106.61 (3) | Ni12—Sn8—Tm1                                | 64.59 (5)  |
| Sn6—Tm2—Ni10                              | 47.67 (3)  | Li12 <sup>i</sup> —Sn8—Tm1                  | 64.59 (5)  |
| Sn4—Tm2—Ni10                              | 89.69 (3)  | Ni12 <sup>i</sup> —Sn8—Tm1                  | 64.59 (5)  |
| Sn4 <sup>i</sup> —Tm2—Ni10                | 161.22 (4) | Ni10 <sup>vii</sup> —Sn8—Tm1                | 146.57 (5) |
| Sn8 <sup>iii</sup> —Tm2—Ni10              | 49.23 (3)  | Sn4 <sup>vii</sup> —Sn8—Tm1                 | 107.97 (3) |
| Sn8 <sup>iv</sup> —Tm2—Ni10               | 107.01 (3) | Tm2 <sup>vi</sup> —Sn8—Tm1                  | 130.45 (2) |
| Sn4 <sup>v</sup> —Tm2—Ni10                | 132.82 (3) | Tm2 <sup>vii</sup> —Sn8—Tm1                 | 130.45 (2) |
| Sn7—Tm2—Ni10                              | 46.61 (3)  | Ni12—Sn8—Sn7 <sup>vii</sup>                 | 56.56 (5)  |
| Ni10 <sup>i</sup> —Tm2—Ni10               | 84.84 (4)  | Li12 <sup>i</sup> —Sn8—Sn7 <sup>vii</sup>   | 131.17 (6) |
| Sn6 <sup>i</sup> —Tm2—Ni11 <sup>i</sup>   | 47.59 (3)  | Ni12 <sup>i</sup> —Sn8—Sn7 <sup>vii</sup>   | 131.17 (6) |
| Sn6—Tm2—Ni11 <sup>i</sup>                 | 105.45 (3) | Ni10 <sup>vii</sup> —Sn8—Sn7 <sup>vii</sup> | 49.92 (3)  |
| Sn4—Tm2—Ni11 <sup>i</sup>                 | 106.85 (3) | Sn4 <sup>vii</sup> —Sn8—Sn7 <sup>vii</sup>  | 120.89 (3) |
| Sn4 <sup>i</sup> —Tm2—Ni11 <sup>i</sup>   | 49.91 (3)  | Tm2 <sup>vi</sup> —Sn8—Sn7 <sup>vii</sup>   | 116.50 (3) |
| Sn8 <sup>iii</sup> —Tm2—Ni11 <sup>i</sup> | 161.30 (4) | Tm2 <sup>vii</sup> —Sn8—Sn7 <sup>vii</sup>  | 59.72 (2)  |
| Sn8 <sup>iv</sup> —Tm2—Ni11 <sup>i</sup>  | 91.14 (3)  | Tm1—Sn8—Sn7 <sup>vii</sup>                  | 110.00 (3) |
| Sn4 <sup>v</sup> —Tm2—Ni11 <sup>i</sup>   | 45.84 (2)  | Ni12—Sn8—Sn7 <sup>vi</sup>                  | 131.17 (6) |
| Sn7—Tm2—Ni11 <sup>i</sup>                 | 133.57 (3) | Li12 <sup>i</sup> —Sn8—Sn7 <sup>vi</sup>    | 56.56 (5)  |
| Ni10 <sup>i</sup> —Tm2—Ni11 <sup>i</sup>  | 86.98 (3)  | Ni12 <sup>i</sup> —Sn8—Sn7 <sup>vi</sup>    | 56.56 (5)  |
| Ni10—Tm2—Ni11 <sup>i</sup>                | 147.13 (5) | Ni10 <sup>vii</sup> —Sn8—Sn7 <sup>vi</sup>  | 49.92 (3)  |
| Sn6 <sup>i</sup> —Tm2—Ni11                | 105.45 (3) | Sn4 <sup>vii</sup> —Sn8—Sn7 <sup>vi</sup>   | 120.89 (3) |
| Sn6—Tm2—Ni11                              | 47.59 (3)  | Tm2 <sup>vi</sup> —Sn8—Sn7 <sup>vi</sup>    | 59.72 (2)  |
| Sn4—Tm2—Ni11                              | 49.91 (3)  | Tm2 <sup>vii</sup> —Sn8—Sn7 <sup>vi</sup>   | 116.50 (3) |
| Sn4 <sup>i</sup> —Tm2—Ni11                | 106.85 (3) | Tm1—Sn8—Sn7 <sup>vi</sup>                   | 110.00 (3) |
| Sn8 <sup>iii</sup> —Tm2—Ni11              | 91.14 (3)  | Sn7 <sup>vii</sup> —Sn8—Sn7 <sup>vi</sup>   | 85.38 (3)  |
| Sn8 <sup>iv</sup> —Tm2—Ni11               | 161.30 (4) | Ni12—Sn8—Tm3                                | 76.27 (5)  |
| Sn4 <sup>v</sup> —Tm2—Ni11                | 45.84 (2)  | Li12 <sup>i</sup> —Sn8—Tm3                  | 76.27 (5)  |
| Sn7—Tm2—Ni11                              | 133.57 (3) | Ni12 <sup>i</sup> —Sn8—Tm3                  | 76.27 (5)  |
| Ni10 <sup>i</sup> —Tm2—Ni11               | 147.13 (5) | Ni10 <sup>vii</sup> —Sn8—Tm3                | 69.76 (5)  |
| Ni10—Tm2—Ni11                             | 86.98 (3)  | Sn4 <sup>vii</sup> —Sn8—Tm3                 | 175.22 (4) |
| Ni11 <sup>i</sup> —Tm2—Ni11               | 82.84 (4)  | Tm2 <sup>vi</sup> —Sn8—Tm3                  | 115.88 (2) |
| Ni11—Tm3—Ni11 <sup>i</sup>                | 92.41 (5)  | Tm2 <sup>vii</sup> —Sn8—Tm3                 | 115.88 (2) |
| Ni11—Tm3—Sn7 <sup>vi</sup>                | 170.17 (4) | Tm1—Sn8—Tm3                                 | 76.81 (3)  |
| Ni11 <sup>i</sup> —Tm3—Sn7 <sup>vi</sup>  | 87.78 (3)  | Sn7 <sup>vii</sup> —Sn8—Tm3                 | 56.26 (2)  |
| Ni11—Tm3—Sn7 <sup>vii</sup>               | 87.78 (3)  | Sn7 <sup>vi</sup> —Sn8—Tm3                  | 56.26 (2)  |
| Ni11 <sup>i</sup> —Tm3—Sn7 <sup>vii</sup> | 170.17 (4) | Ni10—Sn9—Sn9 <sup>ii</sup>                  | 116.16 (5) |
| Sn7 <sup>vi</sup> —Tm3—Sn7 <sup>vii</sup> | 90.37 (3)  | Ni10—Sn9—Sn9 <sup>xiv</sup>                 | 116.16 (5) |
| Ni11—Tm3—Sn6                              | 49.56 (3)  | Sn9 <sup>ii</sup> —Sn9—Sn9 <sup>xiv</sup>   | 94.30 (5)  |
| Ni11 <sup>i</sup> —Tm3—Sn6                | 111.10 (4) | Ni10—Sn9—Tm1 <sup>ii</sup>                  | 168.76 (6) |

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| Sn7 <sup>vi</sup> —Tm3—Sn6                  | 139.03 (3)   | Sn9 <sup>ii</sup> —Sn9—Tm1 <sup>ii</sup>   | 70.64 (3)  |
| Sn7 <sup>vii</sup> —Tm3—Sn6                 | 76.34 (2)    | Sn9 <sup>xiv</sup> —Sn9—Tm1 <sup>ii</sup>  | 70.64 (3)  |
| Ni11—Tm3—Sn6 <sup>i</sup>                   | 111.10 (4)   | Ni10—Sn9—Sn7 <sup>xi</sup>                 | 50.37 (3)  |
| Ni11 <sup>i</sup> —Tm3—Sn6 <sup>i</sup>     | 49.56 (3)    | Sn9 <sup>ii</sup> —Sn9—Sn7 <sup>xi</sup>   | 165.45 (5) |
| Sn7 <sup>vi</sup> —Tm3—Sn6 <sup>i</sup>     | 76.34 (2)    | Sn9 <sup>xiv</sup> —Sn9—Sn7 <sup>xi</sup>  | 88.68 (2)  |
| Sn7 <sup>vii</sup> —Tm3—Sn6 <sup>i</sup>    | 139.03 (3)   | Tm1 <sup>ii</sup> —Sn9—Sn7 <sup>xi</sup>   | 123.61 (3) |
| Sn6—Tm3—Sn6 <sup>i</sup>                    | 88.65 (3)    | Ni10—Sn9—Sn7                               | 50.37 (3)  |
| Ni11—Tm3—Sn4 <sup>v</sup>                   | 47.77 (3)    | Sn9 <sup>ii</sup> —Sn9—Sn7                 | 88.68 (2)  |
| Ni11 <sup>i</sup> —Tm3—Sn4 <sup>v</sup>     | 47.77 (3)    | Sn9 <sup>xiv</sup> —Sn9—Sn7                | 165.45 (5) |
| Sn7 <sup>vi</sup> —Tm3—Sn4 <sup>v</sup>     | 128.566 (19) | Tm1 <sup>ii</sup> —Sn9—Sn7                 | 123.61 (3) |
| Sn7 <sup>vii</sup> —Tm3—Sn4 <sup>v</sup>    | 128.566 (19) | Sn7 <sup>xi</sup> —Sn9—Sn7                 | 85.04 (3)  |
| Sn6—Tm3—Sn4 <sup>v</sup>                    | 87.74 (2)    | Ni10—Sn9—Tm3 <sup>iii</sup>                | 68.89 (5)  |
| Sn6 <sup>i</sup> —Tm3—Sn4 <sup>v</sup>      | 87.74 (2)    | Sn9 <sup>ii</sup> —Sn9—Tm3 <sup>iii</sup>  | 129.93 (3) |
| Ni11—Tm3—Sn8                                | 126.12 (3)   | Sn9 <sup>xiv</sup> —Sn9—Tm3 <sup>iii</sup> | 129.93 (3) |
| Ni11 <sup>i</sup> —Tm3—Sn8                  | 126.12 (3)   | Tm1 <sup>ii</sup> —Sn9—Tm3 <sup>iii</sup>  | 99.87 (3)  |
| Sn7 <sup>vi</sup> —Tm3—Sn8                  | 60.46 (2)    | Sn7 <sup>xi</sup> —Sn9—Tm3 <sup>iii</sup>  | 54.95 (2)  |
| Sn7 <sup>vii</sup> —Tm3—Sn8                 | 60.46 (2)    | Sn7—Sn9—Tm3 <sup>iii</sup>                 | 54.95 (2)  |
| Sn6—Tm3—Sn8                                 | 79.58 (2)    | Ni10—Sn9—Tm1                               | 60.61 (3)  |
| Sn6 <sup>i</sup> —Tm3—Sn8                   | 79.58 (2)    | Sn9 <sup>ii</sup> —Sn9—Tm1                 | 56.25 (3)  |
| Sn4 <sup>v</sup> —Tm3—Sn8                   | 162.20 (3)   | Sn9 <sup>xiv</sup> —Sn9—Tm1                | 110.83 (5) |
| Ni11—Tm3—Sn5 <sup>viii</sup>                | 47.97 (4)    | Tm1 <sup>ii</sup> —Sn9—Tm1                 | 126.90 (2) |
| Ni11 <sup>i</sup> —Tm3—Sn5 <sup>viii</sup>  | 105.23 (3)   | Sn7 <sup>xi</sup> —Sn9—Tm1                 | 109.43 (3) |
| Sn7 <sup>vi</sup> —Tm3—Sn5 <sup>viii</sup>  | 122.60 (3)   | Sn7—Sn9—Tm1                                | 59.51 (2)  |
| Sn7 <sup>vii</sup> —Tm3—Sn5 <sup>viii</sup> | 67.83 (2)    | Tm3 <sup>iii</sup> —Sn9—Tm1                | 113.14 (2) |
| Sn6—Tm3—Sn5 <sup>viii</sup>                 | 88.266 (18)  | Ni10—Sn9—Tm1 <sup>xi</sup>                 | 60.61 (3)  |
| Sn6 <sup>i</sup> —Tm3—Sn5 <sup>viii</sup>   | 150.70 (3)   | Sn9 <sup>ii</sup> —Sn9—Tm1 <sup>xi</sup>   | 110.83 (5) |
| Sn4 <sup>v</sup> —Tm3—Sn5 <sup>viii</sup>   | 63.03 (2)    | Sn9 <sup>xiv</sup> —Sn9—Tm1 <sup>xi</sup>  | 56.25 (3)  |
| Sn8—Tm3—Sn5 <sup>viii</sup>                 | 128.29 (2)   | Tm1 <sup>ii</sup> —Sn9—Tm1 <sup>xi</sup>   | 126.90 (2) |
| Ni11—Tm3—Sn5 <sup>ix</sup>                  | 105.23 (3)   | Sn7 <sup>xi</sup> —Sn9—Tm1 <sup>xi</sup>   | 59.51 (2)  |
| Ni11 <sup>i</sup> —Tm3—Sn5 <sup>ix</sup>    | 47.97 (4)    | Sn7—Sn9—Tm1 <sup>xi</sup>                  | 109.43 (3) |
| Sn7 <sup>vi</sup> —Tm3—Sn5 <sup>ix</sup>    | 67.83 (2)    | Tm3 <sup>iii</sup> —Sn9—Tm1 <sup>xi</sup>  | 113.14 (2) |
| Sn7 <sup>vii</sup> —Tm3—Sn5 <sup>ix</sup>   | 122.60 (3)   | Tm1—Sn9—Tm1 <sup>xi</sup>                  | 76.84 (2)  |
| Sn6—Tm3—Sn5 <sup>ix</sup>                   | 150.70 (3)   | Sn9—Ni10—Sn7 <sup>xi</sup>                 | 79.56 (5)  |
| Sn6 <sup>i</sup> —Tm3—Sn5 <sup>ix</sup>     | 88.266 (18)  | Sn9—Ni10—Sn7                               | 79.56 (5)  |
| Sn4 <sup>v</sup> —Tm3—Sn5 <sup>ix</sup>     | 63.03 (2)    | Sn7 <sup>xi</sup> —Ni10—Sn7                | 119.29 (8) |
| Sn8—Tm3—Sn5 <sup>ix</sup>                   | 128.29 (2)   | Sn9—Ni10—Sn6                               | 124.03 (8) |
| Sn5 <sup>viii</sup> —Tm3—Sn5 <sup>ix</sup>  | 80.44 (2)    | Sn7 <sup>xi</sup> —Ni10—Sn6                | 119.49 (4) |
| Ni11—Tm3—Sn9 <sup>vii</sup>                 | 111.84 (4)   | Sn7—Ni10—Sn6                               | 119.49 (4) |
| Ni11 <sup>i</sup> —Tm3—Sn9 <sup>vii</sup>   | 111.84 (4)   | Sn9—Ni10—Sn8 <sup>iii</sup>                | 132.26 (8) |
| Sn7 <sup>vi</sup> —Tm3—Sn9 <sup>vii</sup>   | 59.24 (2)    | Sn7 <sup>xi</sup> —Ni10—Sn8 <sup>iii</sup> | 76.87 (5)  |
| Sn7 <sup>vii</sup> —Tm3—Sn9 <sup>vii</sup>  | 59.24 (2)    | Sn7—Ni10—Sn8 <sup>iii</sup>                | 76.87 (5)  |
| Sn6—Tm3—Sn9 <sup>vii</sup>                  | 133.565 (16) | Sn6—Ni10—Sn8 <sup>iii</sup>                | 103.71 (7) |
| Sn6 <sup>i</sup> —Tm3—Sn9 <sup>vii</sup>    | 133.565 (16) | Sn9—Ni10—Tm1                               | 75.45 (4)  |
| Sn4 <sup>v</sup> —Tm3—Sn9 <sup>vii</sup>    | 108.72 (3)   | Sn7 <sup>xi</sup> —Ni10—Tm1                | 150.48 (7) |
| Sn8—Tm3—Sn9 <sup>vii</sup>                  | 89.08 (3)    | Sn7—Ni10—Tm1                               | 71.26 (3)  |
| Sn5 <sup>viii</sup> —Tm3—Sn9 <sup>vii</sup> | 64.13 (2)    | Sn6—Ni10—Tm1                               | 65.06 (4)  |
| Sn5 <sup>ix</sup> —Tm3—Sn9 <sup>vii</sup>   | 64.13 (2)    | Sn8 <sup>iii</sup> —Ni10—Tm1               | 132.15 (3) |
| Ni11—Tm3—Ni10 <sup>vii</sup>                | 132.07 (3)   | Sn9—Ni10—Tm1 <sup>xi</sup>                 | 75.45 (4)  |
| Ni11 <sup>i</sup> —Tm3—Ni10 <sup>vii</sup>  | 132.07 (3)   | Sn7 <sup>xi</sup> —Ni10—Tm1 <sup>xi</sup>  | 71.26 (3)  |

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| Sn7 <sup>vi</sup> —Tm3—Ni10 <sup>vii</sup>   | 45.186 (14)  | Sn7—Ni10—Tm1 <sup>xi</sup>                  | 150.48 (7) |
| Sn7 <sup>vii</sup> —Tm3—Ni10 <sup>vii</sup>  | 45.186 (14)  | Sn6—Ni10—Tm1 <sup>xi</sup>                  | 65.06 (4)  |
| Sn6—Tm3—Ni10 <sup>vii</sup>                  | 111.93 (3)   | Sn8 <sup>iii</sup> —Ni10—Tm1 <sup>xi</sup>  | 132.15 (3) |
| Sn6 <sup>i</sup> —Tm3—Ni10 <sup>vii</sup>    | 111.93 (3)   | Tm1—Ni10—Tm1 <sup>xi</sup>                  | 87.31 (5)  |
| Sn4 <sup>v</sup> —Tm3—Ni10 <sup>vii</sup>    | 151.69 (4)   | Sn9—Ni10—Tm2 <sup>xi</sup>                  | 137.40 (2) |
| Sn8—Tm3—Ni10 <sup>vii</sup>                  | 46.11 (3)    | Sn7 <sup>xi</sup> —Ni10—Tm2 <sup>xi</sup>   | 65.00 (3)  |
| Sn5 <sup>viii</sup> —Tm3—Ni10 <sup>vii</sup> | 96.20 (3)    | Sn7—Ni10—Tm2 <sup>xi</sup>                  | 137.87 (7) |
| Sn5 <sup>ix</sup> —Tm3—Ni10 <sup>vii</sup>   | 96.20 (3)    | Sn6—Ni10—Tm2 <sup>xi</sup>                  | 62.75 (4)  |
| Sn9 <sup>vii</sup> —Tm3—Ni10 <sup>vii</sup>  | 42.97 (3)    | Sn8 <sup>iii</sup> —Ni10—Tm2 <sup>xi</sup>  | 62.99 (4)  |
| Ni11 <sup>x</sup> —Sn4—Ni11 <sup>v</sup>     | 120.64 (7)   | Tm1—Ni10—Tm2 <sup>xi</sup>                  | 127.82 (6) |
| Ni11 <sup>x</sup> —Sn4—Ni11                  | 103.86 (4)   | Tm1 <sup>xi</sup> —Ni10—Tm2 <sup>xi</sup>   | 71.45 (2)  |
| Ni11 <sup>v</sup> —Sn4—Ni11                  | 103.86 (4)   | Sn9—Ni10—Tm2                                | 137.40 (2) |
| Ni11 <sup>x</sup> —Sn4—Sn8 <sup>iii</sup>    | 109.77 (4)   | Sn7 <sup>xi</sup> —Ni10—Tm2                 | 137.87 (7) |
| Ni11 <sup>v</sup> —Sn4—Sn8 <sup>iii</sup>    | 109.77 (4)   | Sn7—Ni10—Tm2                                | 65.00 (3)  |
| Ni11—Sn4—Sn8 <sup>iii</sup>                  | 107.99 (5)   | Sn6—Ni10—Tm2                                | 62.75 (4)  |
| Ni11 <sup>x</sup> —Sn4—Tm2                   | 164.54 (4)   | Sn8 <sup>iii</sup> —Ni10—Tm2                | 62.99 (4)  |
| Ni11 <sup>v</sup> —Sn4—Tm2                   | 74.78 (3)    | Tm1—Ni10—Tm2                                | 71.45 (2)  |
| Ni11—Sn4—Tm2                                 | 69.01 (3)    | Tm1 <sup>xi</sup> —Ni10—Tm2                 | 127.82 (6) |
| Sn8 <sup>iii</sup> —Sn4—Tm2                  | 61.91 (2)    | Tm2 <sup>xi</sup> —Ni10—Tm2                 | 84.84 (4)  |
| Ni11 <sup>x</sup> —Sn4—Tm2 <sup>xi</sup>     | 74.78 (3)    | Sn9—Ni10—Tm3 <sup>iii</sup>                 | 68.13 (5)  |
| Ni11 <sup>v</sup> —Sn4—Tm2 <sup>xi</sup>     | 164.54 (4)   | Sn7 <sup>xi</sup> —Ni10—Tm3 <sup>iii</sup>  | 59.65 (4)  |
| Ni11—Sn4—Tm2 <sup>xi</sup>                   | 69.01 (3)    | Sn7—Ni10—Tm3 <sup>iii</sup>                 | 59.65 (4)  |
| Sn8 <sup>iii</sup> —Sn4—Tm2 <sup>xi</sup>    | 61.91 (2)    | Sn6—Ni10—Tm3 <sup>iii</sup>                 | 167.84 (7) |
| Tm2—Sn4—Tm2 <sup>xi</sup>                    | 89.78 (3)    | Sn8 <sup>iii</sup> —Ni10—Tm3 <sup>iii</sup> | 64.13 (4)  |
| Ni11 <sup>x</sup> —Sn4—Tm2 <sup>v</sup>      | 70.41 (4)    | Tm1—Ni10—Tm3 <sup>iii</sup>                 | 122.41 (4) |
| Ni11 <sup>v</sup> —Sn4—Tm2 <sup>v</sup>      | 70.41 (4)    | Tm1 <sup>xi</sup> —Ni10—Tm3 <sup>iii</sup>  | 122.41 (4) |
| Ni11—Sn4—Tm2 <sup>v</sup>                    | 71.55 (4)    | Tm2 <sup>xi</sup> —Ni10—Tm3 <sup>iii</sup>  | 109.00 (4) |
| Sn8 <sup>iii</sup> —Sn4—Tm2 <sup>v</sup>     | 179.53 (4)   | Tm2—Ni10—Tm3 <sup>iii</sup>                 | 109.00 (4) |
| Tm2—Sn4—Tm2 <sup>v</sup>                     | 117.81 (2)   | Sn4 <sup>x</sup> —Ni11—Sn4 <sup>v</sup>     | 120.64 (7) |
| Tm2 <sup>xi</sup> —Sn4—Tm2 <sup>v</sup>      | 117.81 (2)   | Sn4 <sup>x</sup> —Ni11—Sn6                  | 117.99 (4) |
| Ni11 <sup>x</sup> —Sn4—Tm3 <sup>v</sup>      | 63.03 (4)    | Sn4 <sup>v</sup> —Ni11—Sn6                  | 117.99 (4) |
| Ni11 <sup>v</sup> —Sn4—Tm3 <sup>v</sup>      | 63.03 (4)    | Sn4 <sup>x</sup> —Ni11—Sn5 <sup>viii</sup>  | 83.76 (5)  |
| Ni11—Sn4—Tm3 <sup>v</sup>                    | 142.59 (5)   | Sn4 <sup>v</sup> —Ni11—Sn5 <sup>viii</sup>  | 83.76 (5)  |
| Sn8 <sup>iii</sup> —Sn4—Tm3 <sup>v</sup>     | 109.43 (3)   | Sn6—Ni11—Sn5 <sup>viii</sup>                | 121.24 (7) |
| Tm2—Sn4—Tm3 <sup>v</sup>                     | 130.985 (18) | Sn4 <sup>x</sup> —Ni11—Sn4                  | 76.14 (4)  |
| Tm2 <sup>xi</sup> —Sn4—Tm3 <sup>v</sup>      | 130.985 (18) | Sn4 <sup>v</sup> —Ni11—Sn4                  | 76.14 (4)  |
| Tm2 <sup>v</sup> —Sn4—Tm3 <sup>v</sup>       | 71.04 (2)    | Sn6—Ni11—Sn4                                | 100.37 (6) |
| Ni11 <sup>x</sup> —Sn4—Sn4 <sup>v</sup>      | 126.78 (6)   | Sn5 <sup>viii</sup> —Ni11—Sn4               | 138.39 (7) |
| Ni11 <sup>v</sup> —Sn4—Sn4 <sup>v</sup>      | 54.61 (4)    | Sn4 <sup>x</sup> —Ni11—Tm3                  | 154.05 (7) |
| Ni11—Sn4—Sn4 <sup>v</sup>                    | 49.25 (3)    | Sn4 <sup>v</sup> —Ni11—Tm3                  | 69.20 (2)  |
| Sn8 <sup>iii</sup> —Sn4—Sn4 <sup>v</sup>     | 121.54 (3)   | Sn6—Ni11—Tm3                                | 67.24 (4)  |
| Tm2—Sn4—Sn4 <sup>v</sup>                     | 59.64 (2)    | Sn5 <sup>viii</sup> —Ni11—Tm3               | 73.14 (4)  |
| Tm2 <sup>xi</sup> —Sn4—Sn4 <sup>v</sup>      | 116.83 (4)   | Sn4—Ni11—Tm3                                | 129.35 (3) |
| Tm2 <sup>v</sup> —Sn4—Sn4 <sup>v</sup>       | 58.17 (3)    | Sn4 <sup>x</sup> —Ni11—Tm3 <sup>xi</sup>    | 69.20 (2)  |
| Tm3 <sup>v</sup> —Sn4—Sn4 <sup>v</sup>       | 108.24 (3)   | Sn4 <sup>v</sup> —Ni11—Tm3 <sup>xi</sup>    | 154.05 (7) |
| Ni11 <sup>x</sup> —Sn4—Sn4 <sup>x</sup>      | 54.61 (4)    | Sn6—Ni11—Tm3 <sup>xi</sup>                  | 67.24 (4)  |
| Ni11 <sup>v</sup> —Sn4—Sn4 <sup>x</sup>      | 126.78 (6)   | Sn5 <sup>viii</sup> —Ni11—Tm3 <sup>xi</sup> | 73.14 (4)  |
| Ni11—Sn4—Sn4 <sup>x</sup>                    | 49.25 (3)    | Sn4—Ni11—Tm3 <sup>xi</sup>                  | 129.35 (3) |
| Sn8 <sup>iii</sup> —Sn4—Sn4 <sup>x</sup>     | 121.54 (3)   | Tm3—Ni11—Tm3 <sup>xi</sup>                  | 92.41 (5)  |

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| Tm2—Sn4—Sn4 <sup>x</sup>                     | 116.83 (4)   | Sn4 <sup>x</sup> —Ni11—Tm2                  | 135.01 (7) |
| Tm2 <sup>xi</sup> —Sn4—Sn4 <sup>x</sup>      | 59.64 (2)    | Sn4 <sup>v</sup> —Ni11—Tm2                  | 63.75 (3)  |
| Tm2 <sup>v</sup> —Sn4—Sn4 <sup>x</sup>       | 58.17 (3)    | Sn6—Ni11—Tm2                                | 61.53 (3)  |
| Tm3 <sup>v</sup> —Sn4—Sn4 <sup>x</sup>       | 108.24 (3)   | Sn5 <sup>viii</sup> —Ni11—Tm2               | 137.92 (2) |
| Sn4 <sup>v</sup> —Sn4—Sn4 <sup>x</sup>       | 85.36 (4)    | Sn4—Ni11—Tm2                                | 61.07 (3)  |
| Ni12—Sn5—Ni11 <sup>xii</sup>                 | 118.18 (7)   | Tm3—Ni11—Tm2                                | 70.75 (2)  |
| Ni12—Sn5—Tm3 <sup>xii</sup>                  | 137.69 (2)   | Tm3 <sup>xi</sup> —Ni11—Tm2                 | 128.71 (6) |
| Ni11 <sup>xii</sup> —Sn5—Tm3 <sup>xiii</sup> | 58.89 (3)    | Sn4 <sup>x</sup> —Ni11—Tm2 <sup>xi</sup>    | 63.75 (3)  |
| Ni12—Sn5—Tm3 <sup>xiii</sup>                 | 137.69 (2)   | Sn4 <sup>v</sup> —Ni11—Tm2 <sup>xi</sup>    | 135.01 (7) |
| Ni11 <sup>xii</sup> —Sn5—Tm3 <sup>xiii</sup> | 58.89 (3)    | Sn6—Ni11—Tm2 <sup>xi</sup>                  | 61.53 (3)  |
| Tm3 <sup>xii</sup> —Sn5—Tm3 <sup>xiii</sup>  | 80.44 (2)    | Sn5 <sup>viii</sup> —Ni11—Tm2 <sup>xi</sup> | 137.92 (2) |
| Ni12—Sn5—Tm1 <sup>xi</sup>                   | 59.57 (4)    | Sn4—Ni11—Tm2 <sup>xi</sup>                  | 61.07 (3)  |
| Ni11 <sup>xii</sup> —Sn5—Tm1 <sup>xi</sup>   | 138.857 (19) | Tm3—Ni11—Tm2 <sup>xi</sup>                  | 128.71 (6) |
| Tm3 <sup>xii</sup> —Sn5—Tm1 <sup>xi</sup>    | 153.58 (3)   | Tm3 <sup>xi</sup> —Ni11—Tm2 <sup>xi</sup>   | 70.75 (2)  |
| Tm3 <sup>xiii</sup> —Sn5—Tm1 <sup>xi</sup>   | 94.310 (14)  | Tm2—Ni11—Tm2 <sup>xi</sup>                  | 82.84 (4)  |
| Ni12—Sn5—Tm1                                 | 59.57 (4)    | Sn4 <sup>x</sup> —Ni11—Tm2 <sup>v</sup>     | 60.33 (4)  |
| Ni11 <sup>xii</sup> —Sn5—Tm1                 | 138.857 (19) | Sn4 <sup>v</sup> —Ni11—Tm2 <sup>v</sup>     | 60.33 (4)  |
| Tm3 <sup>xii</sup> —Sn5—Tm1                  | 94.310 (14)  | Sn6—Ni11—Tm2 <sup>v</sup>                   | 160.53 (7) |
| Tm3 <sup>xiii</sup> —Sn5—Tm1                 | 153.58 (3)   | Sn5 <sup>viii</sup> —Ni11—Tm2 <sup>v</sup>  | 78.23 (5)  |
| Tm1 <sup>xi</sup> —Sn5—Tm1                   | 78.88 (2)    | Sn4—Ni11—Tm2 <sup>v</sup>                   | 60.16 (4)  |
| Ni12—Sn6—Ni10                                | 111.40 (7)   | Tm3—Ni11—Tm2 <sup>v</sup>                   | 123.78 (4) |
| Ni12—Sn6—Ni11                                | 126.13 (7)   | Tm3 <sup>xi</sup> —Ni11—Tm2 <sup>v</sup>    | 123.78 (4) |
| Ni10—Sn6—Ni11                                | 122.47 (7)   | Tm2—Ni11—Tm2 <sup>v</sup>                   | 104.85 (4) |
| Ni12—Sn6—Tm2 <sup>xi</sup>                   | 134.083 (17) | Tm2 <sup>xi</sup> —Ni11—Tm2 <sup>v</sup>    | 104.85 (4) |
| Ni10—Sn6—Tm2 <sup>xi</sup>                   | 69.57 (3)    | Sn8—Ni12—Sn8 <sup>xi</sup>                  | 126.20 (9) |
| Ni11—Sn6—Tm2 <sup>xi</sup>                   | 70.88 (3)    | Sn8—Ni12—Sn6                                | 113.33 (5) |
| Ni12—Sn6—Tm2                                 | 134.083 (17) | Sn8 <sup>xi</sup> —Ni12—Sn6                 | 113.33 (5) |
| Ni10—Sn6—Tm2                                 | 69.57 (3)    | Sn8—Ni12—Sn5                                | 87.74 (6)  |
| Ni11—Sn6—Tm2                                 | 70.88 (3)    | Sn8 <sup>xi</sup> —Ni12—Sn5                 | 87.74 (6)  |
| Tm2 <sup>xi</sup> —Sn6—Tm2                   | 90.64 (3)    | Sn6—Ni12—Sn5                                | 123.90 (9) |
| Ni12—Sn6—Tm1                                 | 65.63 (4)    | Sn8—Ni12—Sn7 <sup>vii</sup>                 | 75.93 (5)  |
| Ni10—Sn6—Tm1                                 | 66.95 (3)    | Sn8 <sup>xi</sup> —Ni12—Sn7 <sup>vii</sup>  | 75.93 (5)  |
| Ni11—Sn6—Tm1                                 | 135.524 (14) | Sn6—Ni12—Sn7 <sup>vii</sup>                 | 93.61 (7)  |
| Tm2 <sup>xi</sup> —Sn6—Tm1                   | 136.53 (3)   | Sn5—Ni12—Sn7 <sup>vii</sup>                 | 142.49 (8) |
| Tm2—Sn6—Tm1                                  | 74.304 (16)  | Sn8—Ni12—Tm1 <sup>xi</sup>                  | 156.15 (8) |
| Ni12—Sn6—Tm1 <sup>xi</sup>                   | 65.63 (4)    | Sn8 <sup>xi</sup> —Ni12—Tm1 <sup>xi</sup>   | 69.53 (3)  |
| Ni10—Sn6—Tm1 <sup>xi</sup>                   | 66.95 (3)    | Sn6—Ni12—Tm1 <sup>xi</sup>                  | 67.18 (4)  |
| Ni11—Sn6—Tm1 <sup>xi</sup>                   | 135.524 (14) | Sn5—Ni12—Tm1 <sup>xi</sup>                  | 74.18 (5)  |
| Tm2 <sup>xi</sup> —Sn6—Tm1 <sup>xi</sup>     | 74.304 (16)  | Sn7 <sup>vii</sup> —Ni12—Tm1 <sup>xi</sup>  | 127.76 (4) |
| Tm2—Sn6—Tm1 <sup>xi</sup>                    | 136.53 (3)   | Sn8—Ni12—Tm1                                | 69.53 (3)  |
| Tm1—Sn6—Tm1 <sup>xi</sup>                    | 88.94 (3)    | Sn8 <sup>xi</sup> —Ni12—Tm1                 | 156.15 (8) |
| Ni12—Sn6—Tm3 <sup>xi</sup>                   | 79.46 (4)    | Sn6—Ni12—Tm1                                | 67.18 (4)  |
| Ni10—Sn6—Tm3 <sup>xi</sup>                   | 135.290 (16) | Sn5—Ni12—Tm1                                | 74.18 (5)  |
| Ni11—Sn6—Tm3 <sup>xi</sup>                   | 63.20 (3)    | Sn7 <sup>vii</sup> —Ni12—Tm1                | 127.76 (4) |
| Tm2 <sup>xi</sup> —Sn6—Tm3 <sup>xi</sup>     | 72.611 (17)  | Tm1 <sup>xi</sup> —Ni12—Tm1                 | 90.29 (6)  |
| Tm2—Sn6—Tm3 <sup>xi</sup>                    | 134.01 (3)   | Sn8—Ni12—Tm2 <sup>vii</sup>                 | 63.18 (5)  |
| Tm1—Sn6—Tm3 <sup>xi</sup>                    | 144.75 (4)   | Sn8 <sup>xi</sup> —Ni12—Tm2 <sup>vii</sup>  | 63.18 (5)  |
| Tm1 <sup>xi</sup> —Sn6—Tm3 <sup>xi</sup>     | 80.659 (16)  | Sn6—Ni12—Tm2 <sup>vii</sup>                 | 155.17 (8) |
| Ni12—Sn6—Tm3                                 | 79.46 (4)    | Sn5—Ni12—Tm2 <sup>vii</sup>                 | 80.93 (6)  |

|                            |              |   |            |
|----------------------------|--------------|---|------------|
| Ni10—Sn6—Tm3               | 135.290 (16) | Sn7 <sup>vii</sup> —Ni12—Tm2 <sup>vii</sup> | 61.56 (4)  |
| Ni11—Sn6—Tm3               | 63.20 (3)    | Tm1 <sup>xi</sup> —Ni12—Tm2 <sup>vii</sup>  | 126.83 (4) |
| Tm2 <sup>xi</sup> —Sn6—Tm3 | 134.01 (3)   | Tm1—Ni12—Tm2 <sup>vii</sup>                 | 126.83 (4) |

Symmetry codes: (i)  $x, y+1, z$ ; (ii)  $-x+1, -y, -z$ ; (iii)  $-x+1/2, -y, z-1/2$ ; (iv)  $-x+1/2, -y+1, z-1/2$ ; (v)  $-x, -y, -z$ ; (vi)  $-x+1/2, -y+1, z+1/2$ ; (vii)  $-x+1/2, -y, z+1/2$ ; (viii)  $x-1/2, y, -z+1/2$ ; (ix)  $x-1/2, y+1, -z+1/2$ ; (x)  $-x, -y-1, -z$ ; (xi)  $x, y-1, z$ ; (xii)  $x+1/2, y, -z+1/2$ ; (xiii)  $x+1/2, y-1, -z+1/2$ ; (xiv)  $-x+1, -y-1, -z$ .